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Continuum Mechanics-Discrete Defect Modeling and Bubble Raft Simulation of Cracked Specimen Response in Nanoscale Geometries

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ABSTRACT

In a continuation of prior work, a new group of Bragg bubble model experiments have been performed to explore the effects of nanoscale crack size and nanoscale structural geometry on atomically-sharp crack tip dislocation emission behavior. The experiments have been designed to correspond to the theoretical limits that bound the expected crack tip response. Continuum elasticity analyses of these situations have also been carried out, in which the leading-order terms in the Williams expansion (the K and T terms) are determined, and the predictions of these continuum analyses coupled with discrete dislocation theory are compared with the experimental results. The experiments exhibit fascinating changes in crack tip dislocation emission direction with changing crack and structural size, crack location and loading conditions, as well as substantial changes in the magnitude of the resolved shear stress that drives dislocation emission. These changes are predicted well by the continuum elasticity-discrete dislocation model down to extremely small dimensions, on the order of a few atomic spacings. Preliminary experiments were performed with layered and two-atom basis rafts to establish crucial comparisons between theory and experiment that validate the applicability of continuum elasticity theory to make predictions directly related to nanoscale fracture behavior.

INTRODUCTION

The nominal fracture response of a cracked material can be considered to be a competition between cleavage crack growth and the spontaneous emission of blunting dislocations [1]. With nanoscale multilayered geometries this framework indicates potential length-scale-induced material transitions due to high densities of physical boundaries. Novel multilayered structures therefore may exhibit transitional behaviors, through the modification of strength and fracture toughness, that are not experienced on larger scales.

An alternative to discrete lattice calculations, proceeding *ab initio* from quantum mechanics, is the bubble model introduced by Bragg and Nye [2]. The nominal material behavior of the bubble model has been established through the calculation of inter-bubble potential and force law, and is shown to appropriately capture the short-range response of atomic interaction in close-packed materials, most notably copper [3, 4]. The bubble interaction characteristics have made it an attractive means of simulating microscopic phenomena [5-7].

Recently, a study was performed in which sharp cracks were introduced into perfect single crystal rafts to explore the connection between linear elastic fracture mechanics combined with discrete dislocation theory and the crack tip response of a close-packed material down to the nanoscale [8]. This paper is an attempt to further bolster the validity of the theoretical predictions through a new series of experiments.

THEORETICAL FOUNDATION

The radial shear stress is the critical planar stress component for prediction of the edge dislocation emission angle from a sharp crack tip. Under planar loading, edge dislocations will be nucleated at a crack tip and will move away from the tip along the direction of maximum radial shear stress.

It is convenient to use the leading-order terms in the Williams crack tip stress field expansion to calculate the angular orientation that experiences the maximum radial shear stress. If more than the singular leading-order terms are retained, the direction of maximum radial shear stress is a function of radius. Choosing the dislocation core width, $\xi_0 b$, as the appropriate radius, the normalized radial shear stress for a crack that experiences loading of both Modes I and II is

$$\frac{\sigma_{r\theta}}{\sigma}=\frac{K_I}{\sigma\sqrt{2\pi\xi_0 b}}F^{I}_{r\theta}(\theta)+\frac{K_{II}}{\sigma\sqrt{2\pi\xi_0 b}}F^{II}_{r\theta}(\theta)+\frac{T}{\sigma}F^{I(0)}_{r\theta}(\theta) \tag{1}$$

where the universal dimensionless functions, $F_{r\theta}$, are

$$\begin{aligned} F^{I}_{r\theta}(\theta)&=\frac{1}{2}\cos\frac{\theta}{2}\sin\theta \\ F^{II}_{r\theta}(\theta)&=\frac{1}{2}\cos\frac{\theta}{2}(3\cos\theta-1) \\ F^{I(0)}_{r\theta}(\theta)&=-\frac{1}{2}\sin 2\theta. \end{aligned} \tag{2}$$

K_I and K_{II} are the Mode I and Mode II stress intensity factors, respectively, and T is the T-stress for a specific far-field loading. The dislocation core width is chosen as the location to evaluate the shear stress because within this zone the stress fields are nonlinear and the linear elastic solution is invalid; the core width is determined experimentally here, as discussed in the next section.

The stress intensity factors for a specific cracked geometry can be obtained in a straightforward manner [9]. The T-stress, a non-singular constant stress that acts parallel to the crack line can also be calculated in a direct manner. These details are given in a paper in preparation [10]. For very small cracks (on the order of tens of atomic spacings) loaded in Mode I, the critical stress intensity factor for dislocation nucleation can be strongly modified through inclusion of the T-stress [11].

Figure 1 shows the representative crack geometry that will be treated analytically and experimentally. A crack of length $2a$ is parallel to and a distance, h, from a rigid boundary. For boundary displacement or traction normal to the crack K_I, K_{II}, and T have a relatively strong dependence on the normalized distance h/a as $h/a \to 0$:

$$K_I, K_{II} \propto (h/a)^{-3/2}, T \propto (h/a)^{-2}. \tag{3}$$

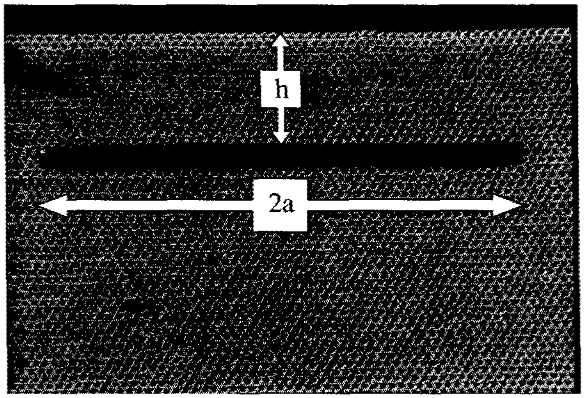


Figure 1. A sharp crack in a single crystal, at a distance, h, from the rigid upper boundary.

EXPERIMENTAL RESULTS

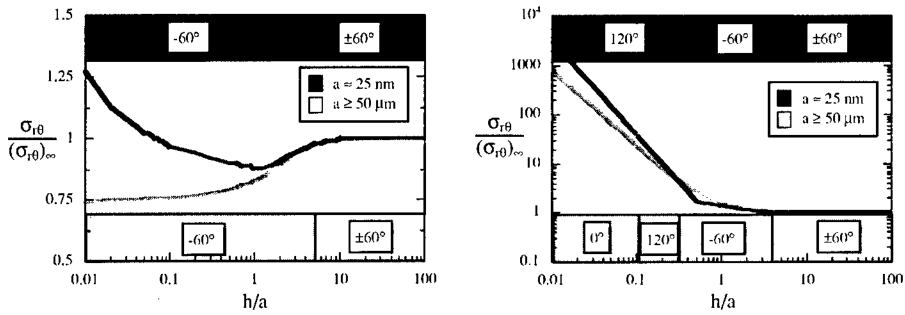
Experiments were performed to explore the qualitative and quantitative shift in dislocation emission from a crack tip as a function of crack location, size, and loading condition. A flat-bottomed, rectangular tray was constructed of polycarbonate to contain the liquid bubble solution. The liquid solution was prepared of soapy water and glycerol in a ratio of 50:1 [12]. Varying the air pressure through the orifice of a small-bore jet controlled the size of the blown bubbles. The bubbles were of uniform size of approximately 1.2 mm in diameter.

Uniform displacement was achieved by fashioning a crack in a perfect bubble raft between two rigid polycarbonate boundaries and then translating the upper polycarbonate boundary in the direction normal or parallel to the stationary boundary. Uniform traction was achieved by constructing a perfect raft around a polycarbonate filament, leaving the upper surface unconstrained. A polycarbonate block was drawn near the free surface to alter the local surface tension and induce normal traction loading. Digital movies of the crack tip processes were taken during the application of the uniform displacement or traction.

In the close-packed structure of the bubble raft, slip will only occur along one of the three equally inclined directions of closely packed rows. With respect to the crack line, this corresponds to emission directions of 0°, ±60°, and ±120°. Therefore, these are the only directions that must be interrogated with Eq. (1) to obtain the maximum radial shear stress.

The soap mixture used for all the bubble experiments exhibited dislocation cores, regions of crystal disregistry, which were spread out over a distance of 5-6 bubble diameters [see e.g. Figure 3] in all cases examined. This dislocation core size was used as a direct material input to solve Eq. (1) for a nanoscale crack. The calculations show that cracks of nanoscale dimension may exhibit different emission behavior than large cracks with identical h/a.

Figures 2(a) and (b) are maps of the predicted dislocation emission directions as a function of h/a for the cases of uniform normal displacement and traction, respectively. The theoretically calculated curves give the maximum shear stress normalized by the maximum shear stress near a crack tip in an infinite body, both for a macroscopic crack and a nanoscale crack. The macroscopic crack is characteristic of the case in which the crack is many orders of magnitude



(a) (b)

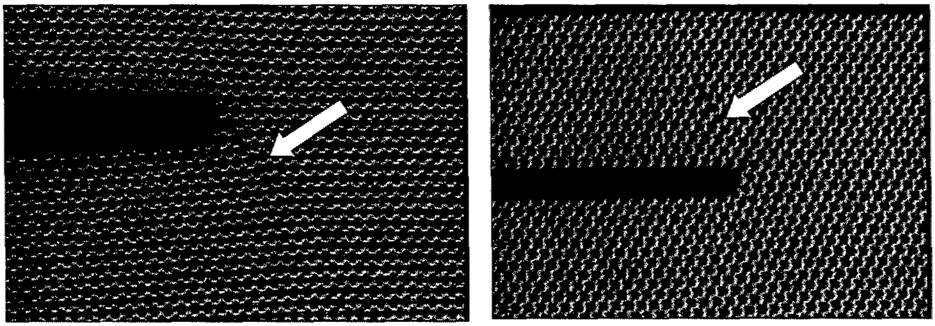
Figure 2. Dislocation emission maps in homogeneous, cracked bubble rafts. The nanoscale crack corresponds to the dark line and the transitions indicated on the upper portion of the plot. The macroscopic crack corresponds to the light line and the lower transitions. Uniform normal (a) displacement and (b) traction.

larger than the atomic spacing and therefore the T-stress is not required to accurately describe the near-tip stress field. Conversely, the T-stress is required for the nanoscale crack where the crack length is of similar order to atomic spacing. The slip direction for which the shear stress is maximized is reported in the plot for each h/a. The dark gray bar at the top and the light gray bar at the bottom indicate the angular orientation with respect to the crack line for which dislocation emission is predicted to occur for the nanoscale crack and macroscale crack respectively.

Corresponding to Figure 2(b) are several uniform normal traction bubble raft simulations. Figure 3(a) shows the case of uniform normal traction for $h/a \approx 2.0$, while Figure 3(b) shows the case for $h/a \approx 0.2$. This transition in emission behavior is expected for a crack with nanoscale dimension as illustrated by the separate emission regimes predicted theoretically for those values of h/a shown in Figure 2(b). Experimental results of uniform normal displacements have been shown previously [8], and are qualitatively similar to the results shown in Figure 3.

Although not shown here, theoretical analyses and experiments have been performed on interfacially-cracked multilayered bubble rafts [13]. The analysis involves a generalization of the homogeneous crack analysis of Eqs. (1) and (2) to the case of a crack on the interface between dissimilar materials. The bubble rafts are constructed of two distinct phases of close-packed bubbles that have different diameters and therefore different elastic moduli. Initial experimentation again shows agreement with theoretical predictions for dislocation emission behavior at a crack tip.

Preliminary investigations of crack tip response have also been made than using bubble rafts that have packing structures other than close-packed. Figure 4 shows the case of a two-atom basis crystal structure. The nature of the soap bubble interactions is essentially the same as a raft constructed of bubbles of one size. However, the dislocation emission response appears to be markedly different. This is due to the different set of allowed slip displacement directions and because the two-atom basis structure has a larger Burgers' vector magnitude and consequently a larger Peierls barrier.



(a) (b)

Figure 3. Crack tip response of bubble rafts experiencing uniform normal traction. Dislocation emission (a) at -60° for $h/a \approx 2.0$ and (b) at 120° for $h/a \approx 0.2$.

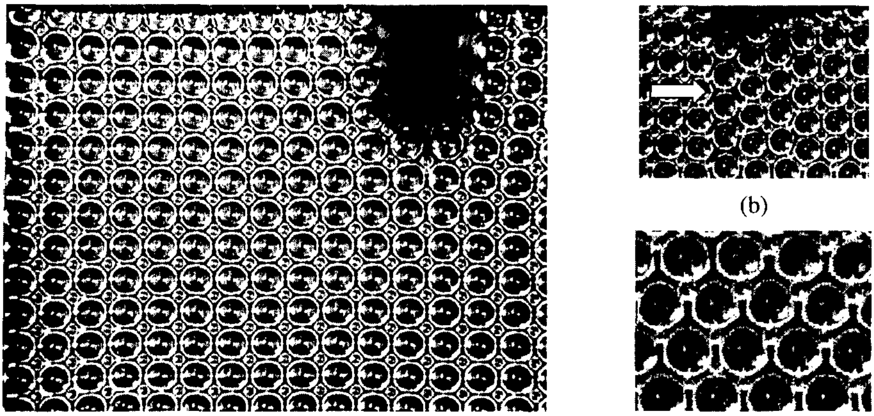
DISCUSSION

As shown through the experiments, most notably the normal traction experiment, omission of the T-stress contribution may give an incorrect prediction for preferred emission direction for nanosized cracks and/or for cracks with nanoscale proximity to a boundary. The case of uniform displacement serves as an upper bound for the response of a crack in a multilayer due to the effectively rigid boundary, while the lower bound was established through the application of uniform surface tractions (perfectly compliant boundary).

A notable feature of the uniform imposed displacement emission map of Figure 2(a) is the substantial change in the stress behavior as the crack length approaches the nanoscale. Instead of exhibiting diminishing shear stress as the crack approaches the boundary (as is the case for the macroscale crack), the maximum shear stress of the nanoscale crack reaches a local minimum for $h/a \approx 1$ and begins to grow as it approaches the boundary. This effect corresponds to a heightened propensity for the emission of a dislocation from the crack tip, and also occurs in the case of nanoscale cracks with $h/a < 0.3$ for imposed normal boundary traction.

Another intriguing implication of this work is the ability of linear elastic fracture mechanics to model the stresses on the nanoscale in such a way that theoretical predictions can be validated in an experimentally repeatable manner. Although an idealized model, continuum elasticity is shown to maintain its predictive capabilities down to a discrete atomic length scale. It may not be appropriate to draw direct parallels between the theory and actual material response in a three-dimensional multilayered material. However, theory and experiment do indicate that a significant transition, with respect to dislocation emission, occurs at a crack tip on the nanoscale.

Certain predictions seem to indicate that materials which behave in a brittle manner in bulk may undergo a transition on the nanoscale for which dislocation emission from a crack tip is preferred over cleavage [13]. These predictions are not testable via the close-packed bubble raft because it is a ductile metal analog. It is hoped that a simple brittle analog will be found that may validate theoretical predictions of a brittle-to-ductile response. The two-atom basis raft, although not a true brittle analog, may be useful as it appears to have a much larger Peierls barrier than its closed-packed counterpart and exhibits elastic response for much larger strains.



(a) (b) (c)

Figure 4. (a) "Sharp" crack in a two-atom basis packing structure that resembles the (001) plane in a "rock salt"-type crystal. (b) Atomic rearrangement along 0° to the crack line. (c) Reordered phase in a two-atom basis packing structure in the most highly strained regions of the raft.

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